Molecular Dynamics Simulations of the Liquid-Vapor Interfacial Region: Cutoff Distance Strategies for Distributed Computing

A.P. Wemhoff [C, S]

Department of Mechanical Engineering, University of California, Berkeley, CA, U.S.A.

V.P. Carey

Department of Mechanical Engineering, University of California, Berkeley, CA, U.S.A.

M. Yue

Department of Mechanical Engineering, University of California, Berkeley, CA, U.S.A.

Knowledge of the thermophysics of liquid-vapor interfaces is important for further study of technological processes involving evaporation and condensation. The thickness of the interfacial region between two phases is on the order of a few molecular diameters, thus requiring analysis on the nanoscale level. This analysis has been performed extensively via computational means such as Molecular Dynamics (MD) and Monte Carlo simulations, where this paper focuses on the former method.

MD simulations of systems of molecules with short-range intermolecular forces often implement creation of an interacting neighbor list for each molecule, where the neighbor list is comprised of molecules that lie within a predefined cutoff distance. An alternative method has been used in this study that divides the simulation domain into regions, designated as 'zones,' where the molecules in each zone only interact with molecules in its own and immediately adjacent zones. The standard and alternative methods have been applied via message-passing multiprocessor programming algorithms to a liquid-vapor system of argon molecules interacting via the Lennard-Jones 6-12 Potential. Our simulations explore the liquid-vapor interfacial region by modeling a liquid region sandwiched between two vapor regions and collecting statistical data across this region. The computational load is allocated to the processors by dividing the zones among processors in a manner to distribute load as evenly as possible. Results show a significant reduction in processing time for the alternative zone method over the conventional neighbor list method for a specified number of processors with no loss of accuracy.

The paper compares results of property profiles across the interfacial region computed using both methods. Localized properties are computed from statistics collected in subregions across the interfacial region. Use of an anisotropic zone cutoff is also explored to more effectively deal with the anisotropic variation of properties in the interfacial region.